



ROBUST CONSTRAINED BLACKBOX OPTIMIZATION WITH SURROGATES

Charles Audet
CORPORATION DE LECOE PLYTECHNIQUE DE MONTREAL

05/21/2015
Final Report

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To: technicalreports@afosr.af.mil

Subject: Final report to Dr. Fariba Fahroo

Grant Title: Robust Constrained Blackbox Optimization With Surrogates

Grant number: FA9550-12-1-0198

Reporting Period: 04/01/2012 to 03/31/2015

Summary of accomplished work:

More and more researchers are getting interested in the field of blackbox optimization. 2012 marked the beginning of new research projects and collaborations.

- Sébastien Le Digabel, who developed the AFORS-funded NOMAD software for blackbox optimization got both tenure and promotion to Associate Professor at the Ecole Polytechnique de Montreal.
- Christophe Tribes continued the development of the NOMAD software. Tribes is from mechanical engineering and his post-doctoral expertise with real MDO problems complements and strengthens our group. His presence extends our collaboration circle to mechanical engineering researchers.
- Our collaboration with A.D. Pelton from chemical engineering, in which we adapted our optimization tools to interact with thermodynamic and properties databases, has lead to three publications in the chemical engineering literature during the reporting period.

- Five undergraduate summer interns spent a semester working on extensions to our NOMAD software.
- Emile Simon, spent a month as a post-doc working on expanding our work on non-smooth optimization to optimal control.
- Andrea Ianni, a PhD Student of the Sapienza University of Rome under the supervision of Stefano Lucidi, spent 6 months in our laboratory to refine the way our method construct poll directions to explore the space of variables. His project lead to important modifications that are currently being tested.
- Our NOMAD C++ software is available at www.gerad.ca/nomad.
- Audet and Le Digabel continue to form highly trained personnel. They are currently supervising 1 MSc student, 7 PhD students, 1 postdoctoral fellow and 1 research professional.
- During the reporting period, a total of 6 MSc and 1 PhD students graduated under the supervision of Audet or Le Digabel.
- Several papers have appeared in top peer reviewed journals. Our papers combine theoretical results, analysis of the limitations of our methods and numerical results on some real engineering problems.
- Professor Audet is organizing a special issue on the topic of Derivative-Free and Blackbox Optimization in the Optimization and Engineering journal.

Personnel Supported:

Faculty: Charles Audet, Sébastien Le Digabel.

Research Staff: Christophe Tribes, Bastien Talgorn.

Students: Mathilde Peyrega, Nadir Amaioua, Amina Ihaddadene and Mathieu Lemyre Garneau.

Summer interns: Stéphane Jacquet, Bénérice Romec, Théophile Lohier, Moustaine Adegbindin and Rachid Cherkaoui.

Archival publications published during reporting period:

Published:

1. C. Audet, S. Le Digabel, and M. Peyrega. Linear equalities in blackbox optimization. *Computational Optimization and Applications*, 61(1):1–23, 2015.
2. E. Bélisle, Z. Huang, S. Le Digabel, and A.E. Gheribi. Evaluation of machine learning interpolation techniques for prediction of physical properties. *Computational Materials Science*, 98, p. 170-177, 2015.
3. B. Talgorn, S. Le Digabel, and M. Kokkolaras. Statistical Surrogate Formulations for Simulation-Based Design Optimization. *Journal of Mechanical Design*, 137(2), p. 021405-1-021405-18, 2015.
4. C. Audet. A survey on direct search methods for blackbox optimization and their applications. In P.M. Pardalos and T.M. Rassias, editors, *Mathematics without boundaries: Surveys in interdisciplinary research*, chapter 2, pages 31–56. Springer, 2014.
5. C. Audet, C.-K Dang, and D. Orban. Optimization of algorithms with OPAL. *Mathematical Programming Computation*, 6(3):233–254, 2014.
6. M.S. Ouali, H. Aoudjit, and C. Audet. Replacement scheduling of a fleet of hydroelectric generators: A case study. *International Journal of Performability Engineering*, 10(6):615–630, 2014.
7. M. Minville, D. Cartier, C. Guay, L.-A. Leclaire, C. Audet, S. Le Digabel, and J. Merleau. Improving process representation in conceptual hydrological model calibration using climate simulations. *Water Resources Research*, 50:5044–5073, 2014.
8. L. Adjengue, C. Audet, and I. Ben Yahia. A variance-based method to rank input variables of the Mesh Adaptive Direct Search algorithm. *Optimization Letters*, 8(5):1599–1610, 2014.
9. C. Audet, A. Ianni, S. Le Digabel, and C. Tribes. Reducing the number of function evaluations in mesh adaptive direct search algorithms. *SIAM Journal on Optimization*, 24(2):621–642, 2014.
10. E.M. Gertz, T. Hiekkalinna, S. Le Digabel, C. Audet, J.D. Terwilliger, and A.A. Schaffer. PSEUDOMARKER 2.0: efficient computation of likelihoods using NOMAD. *BMC Bioinformatics*, 15(47):1–8, 2014.

11. C. Audet, S. Belhaïza, and P. Hansen. A note on bimatrix game maximal selten subsets. *Arabian Journal of Mathematics*, 3(3):299–311, 2014.
12. C. Audet. Ordering 15 marbles with a three-way scale. *The Mathematical Gazette*, 98(542):304–316, 2014.
13. C. Audet, K. Diest, S. Le Digabel, L.A. Sweatlock, and D.E. Marthaler. Metamaterial design by mesh adaptive direct search. In *Numerical Methods for Metamaterial Design*, volume 127 of *Topics in Applied Physics*, pages 71–96. Springer, 2013.
14. A.E. Gheribi, S. Le Digabel, C. Audet, and P. Chartrand. Identifying optimal conditions for magnesium based alloy design using the mesh adaptive direct search algorithm. *Thermochimica Acta*, 559(0):107–110, 2013.
15. C. Audet, C.-K Dang, and D. Orban. Efficient use of parallelism in algorithmic parameter optimization applications. *Optimization Letters*, 7(3):421–433, 2013.
16. S. Alarie, C. Audet, V. Garnier, S. Le Digabel, and L.-A. Leclaire. Snow water equivalent estimation using blackbox optimization. *Pacific Journal of Optimization*, 9(1):1–21, 2013.
17. C. Audet and J. Ninin. Maximal perimeter, diameter and area of equilateral unit-width convex polygons. *Journal of Global Optimization*, 56(3):1007–1016, 2013.
18. C. Audet, P. Hansen, F. Messine, and J. Ninin. The small octagons of maximal width. *Discrete & Computational Geometry*, 49(3):589–600, 2013.
19. A.R. Conn and S. Le Digabel. Use of quadratic models with mesh adaptive direct search for constrained black box optimization. *Optimization Methods and Software*, 28(1), p. 139-158, 2013.
20. C. Audet, J.E. Dennis, and S. Le Digabel. Trade-off studies in blackbox optimization. *Optimization Methods and Software*, 4-5(27):613–624, 2012.
21. C. Audet, S. Belhaïza, and P. Hansen. On proper refinement of bimatrix games extreme nash equilibria. *Automatica*, 2(48):297–303, 2012.
22. A.E. Gheribi, C. Audet, S. Le Digabel, E. Bélisle, C.W. Bale, and A.D. Pelton. Calculating optimal conditions for alloy and process design using thermodynamic and properties databases, the factsage software

and the mesh adaptive direct search (mads) algorithm. *CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry*, 36:135–143, 2012.

23. C. Audet and S. Le Digabel. The mesh adaptive direct search algorithm for periodic variables. *Pacific Journal of Optimization*, 8(1):103–119, 2012.
24. A. Saucier and C. Audet. Construction of sparse signal representations with adaptive multiscale orthogonal bases. *Signal Processing*, 92(6):1446–1457, 2012.

Accepted for Publication:

1. S. Séguin, P. Côté, and C. Audet. Short-term unit commitment and loading problem. To appear in *IEEE Transactions on Power Systems*.
2. R.B. Gramacy, G.A. Gray, S. Le Digabel, H.K.H. Lee, P. Ranjan, G.N. Wells, and S.M. Wild. Modeling an Augmented Lagrangian for Improved Blackbox Constrained Optimization. To appear in *Technometrics* (with discussion).
3. R.B. Gramacy and S. Le Digabel. The mesh adaptive direct search algorithm with treed Gaussian process surrogates. To appear in *Pacific Journal of Optimization*.

Changes in research objectives: None.

The goal of our project remains: The design, analysis, and implementation of optimization tools to aid in making and documenting decisions involving trading off multiple objectives for mixed variable, generally constrained problems with no global smoothness assumptions.

Change in AFOSR program manager, if any: None

Extensions granted or milestones slipped, if any: None

New discoveries, inventions, or patent: None

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FA9550-12-1-0198

Principal Investigator Name

The full name of the principal investigator on the grant or contract.

Charles Audet

Program Manager

The AFOSR Program Manager currently assigned to the award

Dr. Fariba Fahroo

Reporting Period Start Date

04/01/2014

Reporting Period End Date

03/31/2015

Abstract

Our research is about the development of blackbox optimization algorithms, their mathematical analysis and their application, mostly to engineering problems. During the last year of the AFOSR-funded research project we have successfully published research articles in these three areas.

We have extended our Mesh Adaptive Direct Search (MADS) algorithm so that it handles explicit linear equalities using the most appropriate decomposition techniques. We have also completed our research on parameter optimization with a publication in the Mathematical Programming Computation journal. Our work on the identification of statistically important blackbox variables, and on reducing the number of function evaluations, was published. We also introduced different formulations for the surrogate-subproblem, and this work is published in the Journal of Mechanical Engineering journal. Two

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of our papers on augmented Lagrangian and on treed Gaussian processes are accepted for publication, and finally, we have published a literature survey on direct-search methods.

Recent applications of our work include evaluation of machine learning interpolation, simulation-based design optimization, scheduling of a fleet of hydroelectric generators, and calibration of hydrological models.

The PI and CoPi are currently supervising 1 MSc student, 7 PhD students, 1 postdoctoral fellow and 1 research professional. 2 other MSc students graduated during the last year.

Professor Le Digabel got both tenure and promotion to Associate Professor at the Ecole Polytechnique de Montreal. He is also on the organizing committee of the Montreal 2015 CORS-INFORMS conference.

Professor Audet is organizing a special issue on the topic of Derivative-Free and Blackbox Optimization in the Optimization and Engineering journal.

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1) C. Audet, S. Le Digabel and M. Peyrega. Linear equalities in blackbox optimization. Computational Optimization and Applications, 61(1), 1-23, May 2015.

2) E. Béliste, Z. Huang, S. Le Digabel, and A.E. Gheribi, Evaluation of machine learning interpolation techniques for prediction of physical properties. Computational Materials Science, 98, p. 170-177, 2015.

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9) C. Audet, A. Ianni, S. Le Digabel and C. Tribes. Reducing the Number of Function Evaluations in Mesh Adaptive Direct Search Algorithms. SIAM Journal on Optimization, 24(2), 621-642, April 2014.

Refereed papers, accepted for Publication:

10) R.B. Gramacy, G.A. Gray, S. Le Digabel, H.K.H. Lee, P. Ranjan, G.N. Wells, and S.M. Wild, Modeling an Augmented Lagrangian for Improved Blackbox Constrained Optimization. To appear in Technometrics (with discussion).

11) R.B. Gramacy and S. Le Digabel, The mesh adaptive direct search algorithm with treed Gaussian process surrogates. To appear in Pacific Journal of Optimization.

Changes in research objectives (if any):

None

Change in AFOSR Program Manager, if any:

None

Extensions granted or milestones slipped, if any:

None

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, \$K)

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